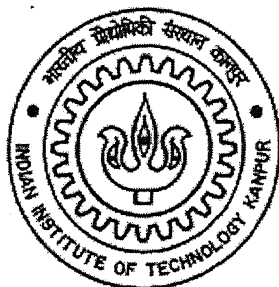


Finite Element Simulation of the Start-Up of Deep Well Wet Oxidation Process

*A Report Submitted to
The Department of Environmental Engineering and Management*

*In Partial Fulfillment of the Requirements for the
Degree of M.Tech in
Environmental Engineering and Management*

*Submitted by
Leena Sharma
Y211711
December 2004*



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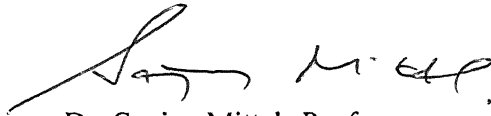
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Certificate

It is certified that the work contained in the thesis titled: *Finite element simulation of start-up of deep well wet oxidation reactor*, by Miss Leena Sharma has been carried out under my supervision.

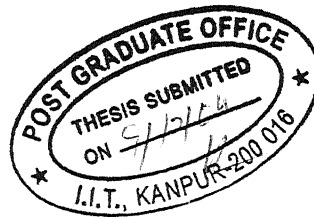


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December 07, 2004



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List of symbols

Subscripts

ud	Interaction between up and down tubes
sd	Interaction between steam and down tubes
F	Fluid
E	Earth

Superscripts

s	Steam Tube
d	Down Tube
u	Up Tube

Greek Symbols

k	Thermal Conductivity of the earth
σ	Heat Transfer Coefficient (per unit length) between the tubes
ρ	Density
$\rho_F^s(x,t)$	Density of fluid in steam tube
ρ_l	Density of liquid
ρ_v	Density of vapour
Λ	The parameter that controls the stability & accuracy of time integration Algorithm.

Other Symbols

x	Linear Coordinate along the tubes in the direction of fluid velocity
H	Depth of the well
h	The penetration depth after which heat transfer is negligible

A	Area of Cross Section
r_o	Radius of the outer casing of the reactor
d	Distance over which heat is added
g	Acceleration due to gravity
\dot{m}	Mass flow rate of the fluid
\dot{m}_F^s	Mass flow rate of the fluid at the entrance of steam tube
\dot{m}_F^d	Mass flow rate of the fluid at the entrance of down tube
\dot{m}_F^u	Mass flow rate of the fluid at the entrance of up tube
$\dot{m}_F^O(t)$	Mass flow rate at the inlet of the steam tube
C_p	Heat Transfer
U	Overall Heat Transfer
\bar{V}	Average Velocity of the fluid
$Q(x,t)$	Heat flux from the reactor tubes per unit length of the tube
$S(x,t)$	Heat added by steam during start-up per unit length of the tube
$T_F^d(x,t)$	Temperature of the Fluid in the down tube
$T_F^s(x,t)$	Temperature of the Fluid in the steam tube
$T_F^u(x,t)$	Temperature of the Fluid in the up tube
$T_E(r,z,t)$	Temperature of the earth
$T_E^0(z)$	Initial Temperature of the earth
$T_s^0(t)$	Temperature at the entry of the steam tube
$(\rho C_p)_E$	Volumetric Heat Capacity of the earth
$(A\rho C_p)_F$	Heat Capacity per unit length of the fluid in the tube
$(A\rho C_p)_P$	Heat Capacity per unit length in the pipe
\hat{h}_F^s	Specific Enthalpy of the fluid in the steam tube
\hat{h}_l	Specific Enthalpy of the liquid

\hat{h}_v	Specific Enthalpy of the vapour
$p_F^s(x, t)$	The Hydrostatic pressure
$\varepsilon_F^s(x, t)$	The Quality of the saturated steam
$p_s^0(x, t)$	Pressure of the fluid at the entry of the steam tube
$\varepsilon_s^0(x, t)$	Quality of the fluid at the entry of the steam tube
Ω_E	The computational domain for the earth
ε_E	The set of elements resulting from the discretization of Ω_E into sub domains Ω_E^e , $e = 1, 2 \dots \text{nel}_E$ where nel_E is the number of elements in Ω_E^e
P^1	The space of the first order polynomials in r^* and z^*
Γ_g	The Dirichlet type boundary
ε_F^i	The set of elements resulting from the finite element discretization of Ω_E into sub domains $(\Omega_F^i)^e$ $e = 1, 2 \dots \text{nel}_F^i$ where nel_F^i is the number of elements in Ω_F^i ; the superscript takes the value s, d & u for steam, down & up tubes respectively
ε_A	Subset of elements in ε_E which are adjacent to the well earth interface
ε	The set of elements for the entire computational domain including the elements in earth and the "pseudo-elements" in the reactor tubes
A	The assembly operator which permutes the elemental level matrices and adds them to global matrices
c_E^e	The elemental level heat capacity matrix
k_E^e	The elemental level conductivity matrix
f_E^e	The elemental level force vector matrix
C	The global heat capacity matrix
K	The global conductivity matrix
F	The global force vector
d	The unknown nodal values of the temperature
v	The unknown nodal values of the time derivative of the temperature

ABSTRACT

Wet air oxidation (WAO) is one of the available technologies for the treatment of aqueous wastewaters containing organic pollutants. It enhances the contact between molecular oxygen and the organic matter to be oxidized. The reactor constructed on this principle contains deep well inside earth, which brings the reactants to the bottom of the reactor and takes out the by-products. The WAO requires certain temperature to start which makes the pre-heating of the reactor is necessary.

This work is a validation of the formulation of the problem and its implementation as proposed in the earlier work by Mittal S. (1990). The earlier work presents a finite element model for the numerical simulation of start-up of the process inside a deep well reactor. It accounts for the heat transfer between the tubes and the heat losses to the surrounding earth and solves the heat conduction equation for earth and heat convection-diffusion for the fluid in the well tubes along with the mass balance of the fluid to find the time dependent temperature profile in the tubes and in the earth. Galerkin and Petrov-Galerkin variational formulation has been used for heat conduction equation of the earth and heat convection-diffusion equation of the well tubes, respectively.

Chapter 1

Introduction

Industrial revolution is a boon or a bane. This is a highly debatable topic. While it has brought upon a major change in human lifestyle in terms of comfort, it has also given birth to a problem that has put a question mark on the existence of mankind itself – pollution. Among the different kinds of pollutions, water pollution is a major one. It has been a very common practice of disposing the industrial wastewater into natural water bodies like rivers, lakes, ponds etc. This polluted water affects the population living around it both directly and indirectly. For this reason, treating wastewater before disposing it into natural water body is necessary. Proper and effective disposal of toxic industrial wastewater has always been a challenge for Environmental Engineers.

Unfortunately, the options for effectively treating the toxic wastewaters and sludge are limited. Alternatives such as dilution, biological (secondary) treatment, physical-chemical (tertiary) polishing, deep-well injection, solar evaporation, incomplete or low-temperature combustion, and low temperature oxidation are not acceptable because the liquid and solid residuals may not meet future disposal criteria. Only two options - deep well-wet oxidation and incineration – are considered as effective as they are capable of destructing toxic organic wastes and sludge almost completely.

Incineration with complete removal of stack discharges and ash stabilization has the potential of burning all organic material completely. But it has certain problems: (a) high construction and operating costs; (b) requires exceedingly high temperatures and complete mixing with assured detention; (c) generally limited to high concentrations of organic wastes in the fire box; (d) elaborate treatment trains involving considerable redundancy for treating stack gases, handling of ash and stack gas treatment streams; and (e) public resentment toward incineration of any kind.

The deep well-wet oxidation process has the potential to achieve many of the desired objectives. It utilizes the unusual property of water of being an excellent solvent at high temperature and pressure. At high temperature and pressure, the solubility of inorganic salts is greatly reduced and the organic compounds are converted to harmless carbon dioxide and water. The kinetics of the process is controlled by reaction rates and not mass transfer. Relatively low waste concentrations can be treated due to efficient heat recovery. The environment is protected because the deep-well concept provides a totally enclosed treatment unit. Nothing is injected into the surrounding earth mass, left on the ground, or released into the atmosphere that is objectionable.

1.1 Physical description of the system

Deep well-wet oxidation is based on the use of a reactor vessel enclosed within drilled and cased wells. The design depth of the well may typically range from 1,524 m to 3,658m (5,000ft to 12,000ft). The reactor consists of a series of concentric tubes hung inside the earth from a surface platform. Fig 1.1 shows the configuration of a Deep Well Oxidation Reactor.

The present work is a validation of the earlier work [1] done by Mittal S. So, the various configurations of the reactor and the parameters of study are kept same. In the original work, the reactor was assumed to have 4 concentric tubes. The detailed description of the reactor configuration is as follows. The concentric tubes, if we move from centre to radially outward direction, are known as steam tube, oxygen tube, down tube and the up tube. The steam tube brings hot steam or water to warm up the reactor. Down tube, as the name suggests takes the sludge down for the oxidation. Oxygen tube carries oxygen and the up tube takes all the residue of the reaction out. All the tubes end up in a common chamber called as reaction chamber. Reaction chamber is the place where the wastewater or sludge and oxygen get mixed and oxidation takes place.

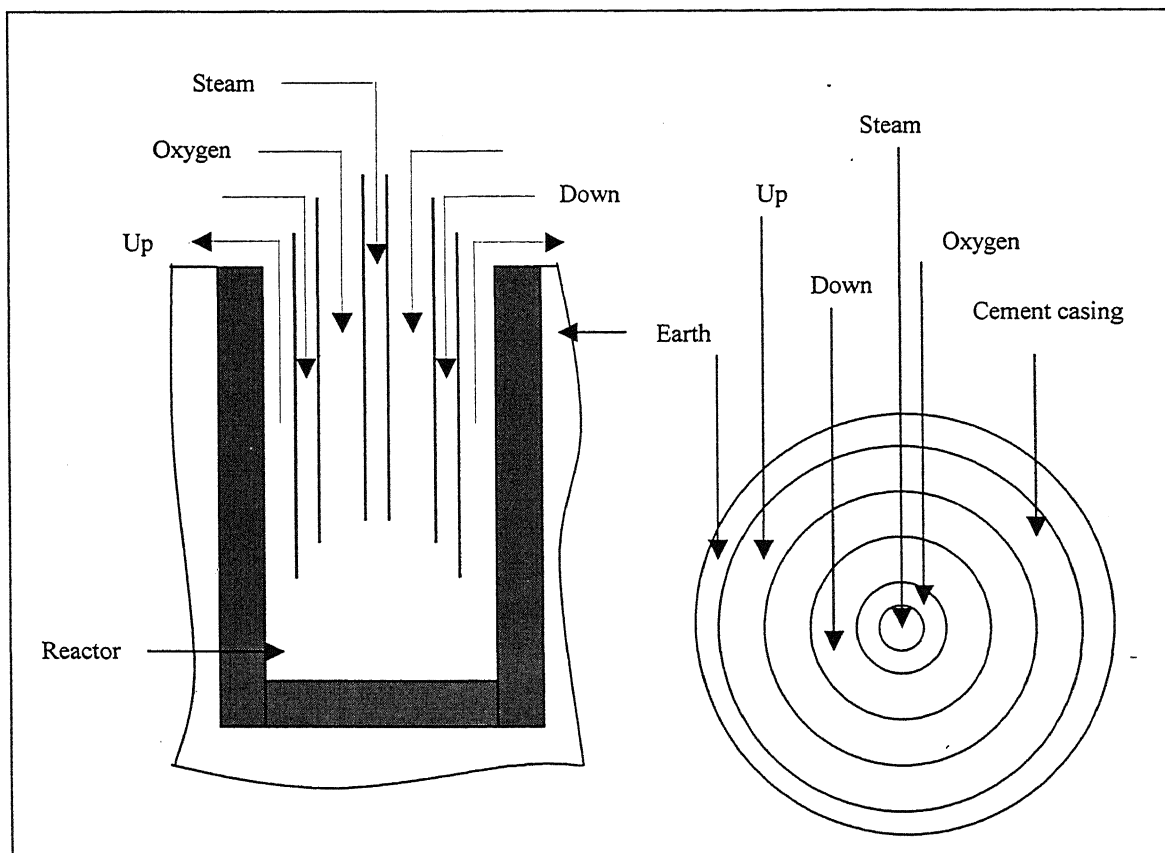


Fig 1.1: Schematic setup of a Deep Well Reactor

The chamber is designed in such a way that the influents get sufficient time for getting oxidized under high temperature and pressure conditions. The outer most tube and the reactor are provided with multi-layered cement casing to prevent any possible seepage of toxic wastewater into the underground waterbed and thus provide extra safety from any possible contamination of underground usable natural water resource.

There are many advantages of using deep well wet-oxidation. Since the water is introduced under a high pressure, the need for the high-pressure liquid pumps, heat exchangers and pressure-reducing methods that appear to be necessary for the aboveground systems, is eliminated. The operation of reactor is very economic as normally a single pass is

sufficient to provide 99.99 to 99.9999% removals of organic substances. Moreover it has sufficient flexibility that it can be operated at a wide range of operating conditions. If high destruction efficiencies are required, the reactor could be operated at low flow rates to provide sufficient reaction time for 99.99% destruction of organic compounds. If less destruction is necessary (80% COD removal), then the same reactor could process wastes at high volumetric flow rates. Lastly, since the reactor is totally enclosed, underground, compact and controlled; safety is inherent in its design.

1.2 Applicability of the process

The Deep Well Oxidation systems are applicable to a wide range of waste materials that include municipal primary, secondary, and mixed sludge; industrial sludge; high strength organic wastes; toxic liquid wastes; and solid hazardous wastes. These systems are designed to provide the desired temperature and density for the required reaction time.

1.3 The Process

The oxidation process cannot start at any temperature so the reactor must be preheated to the desired temperature. In the present model, high-pressure steam or water is injected through the steam tube for preheating. Hot oil can also be used for heating the reactor.

Steam condenses due to heat exchange between steam tube and down tube and gets mixed with the down stream flow from the down tube in the reaction chamber. The oxygen supply is kept off during the start up process as no reaction takes place.

Absence of any flow in oxygen tube results in a very small heat transfer coefficient between the steam and down tube. This prevents the steam from condensing entirely before reaching the bottom. The mixed stream goes out through the up tube. Similarly when the hot

water is used for start up, heat transfer takes place from down tube to up tube, which heats up the reactor tubes.

Steam or water supply is switched off as soon as the initiation temperature of the reaction is achieved. In this model no extra pressure is applied as the hydrostatic pressure provides the sufficient pressure for the reaction. Once the desired temperature is achieved for start up, steam or hot water supply is switched off and oxygen supply is switched on for initiation of the reaction. Oxidation reaction, being exothermic in nature, fuels the further reaction between the sludge and the oxygen. Oxygen, at such high temperature and pressure conditions, mixes completely with water and organic materials, and with a near zero surface tension oxygen can penetrate minute pores. Thus, organic materials under such conditions can be oxidized to CO_2 and H_2O very rapidly.

1.4 The Finite Element Model

For solving the problem numerically, several assumptions have been made:

- Since the diameter of the tube is very small compared to the length of the tube, the temperature variation in radial and azimuthal direction has been neglected. So temperature remains uniform across a given cross - section and varies axially only. With this assumption, it is fair enough to assume the tubes to be one-dimensional. This automatically reduces the 3D problem to a 2D problem.
- All the tubes are assumed to be frictionless. So the pressure in steam tube is assumed to be caused by hydrostatic head only.

The model simultaneously solves the convection heat equations for all the tubes, conduction heat equation for the earth, mass balance equation of the fluid along with appropriate boundary conditions (discussed later) to find the temperature profile of the tubes and the earth. Since the fluid flow is one dimensional, Navier-Stokes equations are not solved for

determining the velocity field. The Petrov-Galerkin formulation has been used for spatial discretization of convection heat equation of the tubes to avoid any spurious node-to-node oscillations in the solution. The heat conduction equation for earth has been discretized spatially using regular Galerkin formulation. Predictor – Multicorrector time algorithm has been used to solve the set of linear algebraic equations obtained from finite element discretization. The details of the model are discussed in later chapters.

Chapter 2

The Wet Air Oxidation Process

In Wet Air Oxidation aqueous waste is oxidized in the liquid phase at high temperatures (400-573 K) and pressures (0.5-20 MPa) in the presence of an oxygen containing gas (usually air). The basic idea of the process is to enhance contact between molecular oxygen and the organic matter to be oxidized. High temperature conditions convert the organic matter to carbon dioxide and water. The liquid phase is maintained by high pressure, which also increases the concentration of dissolved oxygen (COD) and thus the oxidation rate. Typical conditions are 200-325 °C for temperatures, 50-175 bars for pressure and 1 h for the residence time; the preferred COD load ranges from 10 to 80 kg/m³.

2.1 Objective of the process

It is an enclosed process, with a limited interaction with the environment. The process can treat any kind of organic aqueous waste that are too dilute to treat economically, even toxic wastes which can not be treated biologically, produced by various branches of industrial activity, or it can be coupled with a biological treatment facility to eliminate the sludge. WAO is one of the few processes that does not turn pollution from one form to another, but really make it disappear. This process has been used under mild conditions that alters molecular structures and improve biodegradability in spite of a limited COD reduction, but, usually, it is run under conditions that give almost complete oxidation of the organic matter and that can allow mechanical power generation because the reaction is exothermic. It has been established that the energy self-sufficiency is obtained provided that the COD load exceeds 12-15 kg/m³.

2.2 The Deep Well Wet Oxidation Method (DWWO)

The deep well process employs wet oxidation method and is carried out in a vertical reactor buried in the ground. The reactor consists of concentric tubes of length up to 1500 meters or more suspended in a conventionally drilled and cased well. The waste enters the reactor at the surface and flows down the center tube, which is referred to as the down tube or down comer. In the reaction zone, which is approximately the bottom 10-20 per cent of the reactor, the waste stream and oxygen are brought together at high pressure and elevated temperature. Organic oxidation is initiated spontaneously at these conditions. Once initiated the exothermic reaction, combined with countercurrent heat exchange, fuels the process. The products leave through the outer annulus or up tube and exit the reactor at the surface.

2.2.1 Purpose of the Well

The purpose of the well is four-fold:

- 1) To achieve the desired pressure in the reaction zone by the hydrostatic head.
- 2) To allow large surface area for counter-current heat exchange between the descending reactants and ascending products so that the reactor can operate auto thermally (except during start-up and shut-down).
- 3) To use the natural insulating properties and temperature gradients in the rock to minimize heat losses from the reactor.
- 4) To minimize material requirements by taking advantage of the balance between the earth pressure outside and the reactor pressure in the interior.

2.2.2 Advantages of Deep Well configuration

- 1) *Safety*: The pressurized heat exchanger/reactor is located below ground in a steel-cased well. Catastrophic failure of the reactor/heat exchanger will not result in a safety risk to operating personnel or other people in the surrounding area. No Carbon Monoxide or NO_x is produced during oxidation. There is no threat of air and dust emission whatsoever because of its inherent closeness. The behavior of the reactor is always predictable because the mechanism of energy absorption is well known.
- 2) *Simplicity of design and construction*: The reactor serves as the pressurization, heat exchanger and reaction vessel which eliminates recycling of supercritical water or use of high pressure, high temperature heat exchangers. The unit is constructed of threaded tubular pipes.
- 3) *High thermodynamic efficiency*: The counter flow heat exchanger design enables the process to operate autogenically with a waste having a heat value as low as 1.2×10 J/kg (50 Btu/lb).
- 4) *Broad operating range*: The reactor is not confined to a single operating design point. Because of the large size of the reactor and the thermodynamic efficiency of the process, the unit can operate at different flow rates, waste strengths, and operating temperatures.
- 5) *Reduced pump horsepower*: Hydrostatic head can produce the needed pressures.
- 6) *Earth serves as an insulator*: Heat loss is relatively slow.
- 7) *Stability of operating conditions*: The reactor volume is large.

- 8) *Low operating cost:* The processing cost for a deep well reactor in USA is roughly 10 cents per gallon. This is the lowest operating cost among all the available options.

2.2.3 Operational Flexibility of DWWO

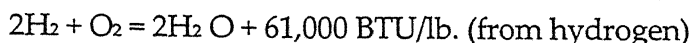
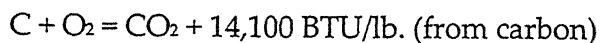
Despite being quite bulky, Deep Well Wet Oxidation process is flexible in operation. The process can be customized very easily, without much change in design of the reactor, for a given set of conditions. The process has following operational flexibilities:

- 1) The pH condition in the reaction chamber can be changed from pH 2 to pH 8.
- 2) The pH acidification can be by sulfuric acid or carbon dioxide gas mix in any proportion.
- 3) The temperature in the reaction chamber can be set anywhere between 200F to 500 F.
- 4) The reaction time can be readily changed from 2 seconds to five minutes.
- 5) The flow rate can be varied 10 to 1 from a nominal rate of 5 ft per second.
- 6) The concentration of suspended solids can vary from 0.01% to 14%.
- 7) The reactor vessel can be cleaned while in service.

2.3 Deep Well Wet Oxidation Process and Above the Ground Wet oxidation Process

For both "top-of-the-ground" and "in-ground" processes, the following general principles of wet oxidation apply:

- 1) The combustion reaction releases heat according to the following equations:



- 2) The combustion occurs in the aqueous phase.
- 3) The heat of vaporization is conserved since the pressure in the vessel is always greater than the vapor pressure of the liquid waste at the oxidation temperature.
- 4) The rate of oxidation is a function of temperature and characteristics of the waste.
- 5) The degree of oxidation is a function of temperature and detention time.

Apart from the principles stated above, the following process requirements must be satisfied for both "in-ground" and "top-of-the-ground" systems, and must be cost effective:

- 1) Presence of organic combustibles.
- 2) Provision of high-pressure liquid,
- 3) Provision of high-pressure source of oxygen; either pure oxygen or air,
- 4) Effective heat exchange (for dilute i.e. less than 200 BTU/lb. waste),
- 5) High-pressure reactor vessels with sufficient liquid detention time for the oxidation reaction to take place (20-30 minutes for sub critical, 1-5 min for supercritical).

2.3.1 Advantages of Deep Well Wet Oxidation Method over above the ground methods

Listed below are important advantages of deep well wet oxidation systems over equivalent units that are constructed on top of the ground:

- 1) *Use of Hydrostatic Head:* The use of hydrostatic head of the reactor allows achieving the necessary reaction pressure by only circulating against the frictional head loss of the downdraft and updraft. This saves from 60-90% of the pumping cost, while significantly reducing the capital and maintenance cost of high-pressure pumps. This inherent process advantage also permits the deep well reactor configuration to process abrasive or other slurry wastes that cannot be reliably and economically pumped to extremely high pressures by top-of-the-ground system.

- 2) *Combined Reactor and Heat Exchangers:* Because of the concentric tubular deep well configuration the reactor acts as both the reaction vessel and the heat exchanger, thus eliminating the need for a separate external high-pressure tube-in-tube heat exchanger. The concentric tubular design of a typical 5000' reactor vessel provides excess heat exchanger capacity with nearly equal pressure on each side of the downdraft tube thereby reducing the cost of the downdraft/heat exchanger over top-of-the-ground external heat exchangers. For example, a separate heat exchanger would have to have 10,000 feet of 3" O.D. tubing of hastelloy material to be thermally equivalent to the deep well reactor "built-in" heat exchanger. Top-of-the-ground tube-in-tube heat exchangers encompass 180-degree bends every 40 feet. These are expensive and have been shown to be extreme points of erosion due to welded construction with un-annealed welds for the 180-degree bends.
- 3) *Natural Insulating Properties of the Earth and Use of Available Thermal Gradient:* Thermal gradient provides a free 50-100 degrees F temperature increase for a typical 5000' reactor thereby allowing a more dilute waste to be treated. Additionally, the thermal insulating properties of the earth provide an excellent natural insulator for the deep well reactor. The long-term storage of heat also reduces the heat required for startup after non-routine shutdowns, and provides potential for energy recovery after the useful life of the waste treatment project.
- 4) *Greater Thermal Efficiency:* The greater thermal efficiency of the deep well reactor permits the treatment of a much more dilute organic stream than a top-of-the-ground system does without the use of a large heat exchanger or other methods to recover generated energy. Deep well reactor can operate with a minimum influent organic strength of 120 BTU/lb. compared to 350-450 BTU/lb. for top-of-the-ground sub critical reactors and 350 BTU/lb. for top of-the-ground supercritical reactors. The inherent greater thermal efficiency of these reactors, exhibit a much more

pronounced economic advantage for super critical application of low BTU wastes since the top-of-the-ground supercritical systems must employ recycling of supercritical fluid or employ expensive high pressure heat exchangers to recover heat. For example, a top-of-the-ground supercritical reactor treating a 10% organic (high strength, 1,750 BTU/lb.) waste requires a 50% recycle of supercritical fluid. This doubles the reactor vessel size for the same reactor detention time. For a dilute waste stream (2% organic with 350 BTU/lb. heating value), a 7,000-psi tube and shell heat exchanger of 1,000 to 1,800 SF is required for an 1,100 degree F reactor operating with supercritical water at a density of 10 lbs/CF.

5) *Fouling Potential:*

- (a) Elimination of topside heat exchangers, which cannot operate in 2-phase mode (gas and liquid), is possible with temperatures (300 degrees F). This low temperature oxidation with sufficient oxygen availability, eliminates char formation and associated fouling from char formation in the reactor vessel/heat exchanger.
- (b) Comparatively low differences in temperature between reactor vessel influent and effluent means fouling from salts (calcium sulfate and calcium carbonate) that are inversely soluble with temperature are not as severe as with above ground units utilizing heat exchangers.

6) *Erosion/Corrosion:*

- a) Use of straight pipe with no bends eliminates erosion problems with U-bends in tube and shell heat exchangers.
- b) Use of premium-threaded joints in the reactor vessel eliminated weld affected areas in reactor pipe that are susceptible to corrosion. All reactor pipes used are in fully annealed conditions to minimize stress corrosion cracking problems. The

bottom 100' plus or minus is made of extra thickness material to give extra erosion resistance.

- c) Lower reactor vessel heat exchanger temperature differentials reduce inorganic fouling over top-of-the-ground heat exchangers.

7) *Broad Operating Range of Reactor Vessels:*

- a) Reactor vessels can be designed to operate over a 100% change in waste strength or flow rate to accommodate changes in reactor feed strength and volume.
- b) Low volume, high strength wastes can be treated successfully in reactor vessels.
- c) Due to continuous nature of reactor vessel/heat exchanger and long oxidation zone in the process, fouling effects, or change in oxidation rate of waste have less effect than with an above ground reactor with separate reaction vessel. For example, in a 5,000 feet reactor vessel, the upper 1/2 of the reactor, when it is clean, operates mainly as a heat exchanger, while the lower 1/2 operates as the reactor vessel. As the heat exchanger portion of the reactor vessel becomes fouled, the reaction zone moves downward into the reactor and, if the flow rate remains steady, the bottom hole temperature rises and the waste destruction efficiency remains complete.

8) *Safety:*

- a) High-pressure reaction vessel/heat exchangers are located below ground in steel cased well. Catastrophic failure of reactor/heat exchanger will not result in safety risk to operating personnel or other people in surrounding area.
- b) If leakage from reactor or catastrophic failure from reactor occurs, all leakage is contained in cased well and is not release to the environment.
- c) If a dangerous situation arises, reactor and well can be flushed out and the material can be stored to prevent its immediate release to the environment.

- 9) *Less Space Requirements:* The deep well reactor vessel technology requires approximately 1.5 acres for an 80 DT/day reactor. This is approximately 1/5 the area required for commonly used alternative technologies.
- 10) *No Gaseous Emissions:* The reactor vessels produce no odors or gaseous emissions that require EPA permits, no NO_x, no CO.

2.3.2 Limitations of Deep Well Wet Oxidation

- 1) It must have at least 25 tons of common organic materials to process during any 24-hour period, or 50 gallons per minute. It varies depending on the actual material.
- 2) The reactor cannot be built within any strata that are subjected to displacement. These include salt domes and the crossing of a seismic fault line.
- 3) The reactor is not portable in the sense that it is not truck mounted. It is relocate able and is designed for a twenty-year life. About fifteen percent of a typical capitalization cost would be lost to the abandoned cased housing chamber if no beneficial use for it can be defined. Suggested uses include mineral extraction and radioactive wastes internment.
- 4) The reactor waste stream must not be so dilute compared to its volume as to fail to provide enough heat energy for both strata heat losses and the terminal temperature difference between the water entering the reactor and the water leaving the reactor. The lower limit appears to be 0.3 percent of organics in water with flow rates of 1500 gallons per minute. Heat shortfall requires added energy.
- 5) The reactor is limited by existing metallurgy to avoid peak operating temperatures in excess of 750°F if significant salts are present in the water stream. Even at cooler temperatures salt concentrations of 10,000 parts per million are suggested to be avoided or diluted.

- 6) When operating in an Oxidation mode the reactor feed should be limited to fewer than 9% of suspended materials in water. There are two considerations in this limitation. The first is the initial viscosity may be too great when dealing with sludge and result in too much pressure drop in the downdraft, which is counter to the preferred engineering. The second consideration is the release of too much heat energy in relation to the available water. Water is the principal heat-absorbing buffer. There is an operating mode where the excess heat may be converted to electric power or high-pressure heated process water but these are very special design cases.

2.4. Types of Deep Well Wet Oxidation Method

The deep well wet oxidation method is of two types:

- 1) Sub critical deep well wet oxidation method
- 2) Supercritical deep well wet oxidation method

2.4.1 Comparison between Sub critical and Supercritical Deep-Well Reactor Designs

The reactors based on the two processes have corresponding names. The design parameters and the optimum operating conditions for the two types of reactors differ significantly. *Table 2.1* presents a comparison between basic design parameters of the two types of reactors.

Parameter		Sub critical Reactor	Supercritical Reactor
Well Depth	-m	1200-1700	2400-3658
	-ft	4000-5500	8000-12000

<i>Temperature</i>	<i>°C</i>	260-320	400-510
	<i>°F</i>	500-600	750-950
<i>Pressure</i>	<i>KN/m²</i>	10000-14000	22000-31000
	<i>Psia</i>	1500-2300	3200-4500
<i>Detention time min</i>		30-40	0.1-2.0
<i>COD removal (%)</i>		80-85	100
<i>Oxidant</i>		Oxygen gas	Oxygen gas
<i>Injection point</i>		Lower ½	Lower 1/20
<i>velocity</i>	<i>m/s</i>	1.2-2.7	1.5-4.6
	<i>Ft/s</i>	2-9	5-15
<i>Applicability</i>		Sludge, organic & toxic wastes	All organic wastes
<i>Waste Destruction Efficiency</i>		Organic species dependent: 80-99%	99.99%

Table 2.1: Comparison between Sub & Super Critical Reactors

Chapter 3

Problem Statement

The aim of this study is to determine the temperature of the fluid in all the reactor tubes and the earth surrounding the reactor and below it during the start-up of the reactor. Further, we want to study the heat transfer from the tubes to the earth. This is important as the reactor may explode if the temperature of the reactor exceeds the safe limits.

In this chapter all the governing equations and the boundary conditions needed to solve for the desired temperature profile in all the tubes and earth are discussed.

3.1 Governing Equations

The governing equations for the model are determined by the heat balance of the fluid in the reactor tubes and the earth and the mass balance of the fluid in the reactor tubes.

Since the reactor tubes are cylindrical, the cylindrical coordinates would be the most natural coordinate system to work with. Given that the computational domain is symmetric in angular direction, it has been assumed that there is no angular variation in the temperature of the earth. Thus the standard Heat Conduction Equation in 2D with constant material properties gives the two dimensional heat balance equation for the temperature of earth:

$$(\rho C_P)_E \frac{\partial T_E}{\partial t} = \kappa \left[\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial T_E}{\partial r} \right) + \frac{\partial^2 T_E}{\partial z^2} \right] \quad (1)$$

Solving for the temperature of a flowing fluid usually requires the velocity of the fluid, which can be found by solving the Navier-Stokes equation for fluid flow. We have

The heat balance equation for the down and up tubes are given by

$$\left[(A\rho C_P)_p^d + (A\rho C_P)_F^d \right] \frac{\partial T_F^d}{\partial t} + \left(\dot{m} C_P \right)_F^d \frac{\partial T_F^d}{\partial x} - (\sigma U)^{sd} (T_F^d - T_F^s) - (\sigma U)^{ud} (T_F^d - T_F^u) = S, \quad 0 \leq x \leq H \quad (5)$$

$$\left[(A\rho C_P)_p^u + (A\rho C_P)_F^u \right] \frac{\partial T_F^u}{\partial t} + \left(\dot{m} C_P \right)_F^u \frac{\partial T_F^u}{\partial x} + (\sigma U)^{ud} (T_F^u - T_F^d) = Q, \quad H \leq x \leq 2H \quad (6)$$

To ensure the mass continuity at the reactor, the following equation is used.

$$\dot{m}_F^u(t) = \dot{m}_F^d + \dot{m}_F^s(H, t) \quad (7)$$

This equation is used to determine the mass flow rate in the up tube. The mass flow rate of the down tube is considered as a constant.

3.2 Thermodynamic Relations

The governing equations described above cannot be solved completely (with given boundary conditions) because the enthalpy and density terms in the equations are functions of temperature and/or pressure. So we need the proper thermodynamic relations. For single phase the enthalpy and density are function of both temperature and pressure.

$$\hat{h}_F^s = \hat{h}_F^s(T_F^s, p_F^s) \quad (8(a))$$

$$\rho_F^s = \rho_F^s(T_F^s, p_F^s) \quad (8(b))$$

Using the definition of complete derivative, equation 8(a) can be differentiated with respect to time and the 1D space coordinate to get

$$\frac{\partial \hat{h}_F^s}{\partial t} = \left(\frac{\partial \hat{h}_F^s}{\partial T_F^s} \right)_{p_F^s} \left(\frac{\partial T_F^s}{\partial t} \right) + \left(\frac{\partial \hat{h}_F^s}{\partial p_F^s} \right)_{T_F^s} \left(\frac{\partial p_F^s}{\partial t} \right) \quad (9(a))$$

$$\frac{\partial h_F^s}{\partial x} = \left(\frac{\partial h_F^s}{\partial T_F^s} \right)_{p_F^s} \left(\frac{\partial T_F^s}{\partial x} \right) + \left(\frac{\partial h_F^s}{\partial p_F^s} \right)_{T_F^s} \left(\frac{\partial p_F^s}{\partial x} \right) \quad 9(b)$$

Now using 9(a), 9(b) and (4), the heat balance equation for steam tube for a single-phase fluid can be modified to

$$\left[(A\rho C_p)_p^s + A_F^s \rho_F^s \left(\frac{\partial \hat{h}_F^s}{\partial T_F^s} \right)_{p_F^s} \right] \frac{\partial T_F^s}{\partial t} + \dot{m}_F^s \left(\frac{\partial \hat{h}_F^s}{\partial T_F^s} \right)_{p_F^s} \frac{\partial T_F^s}{\partial x} + (\sigma U)^{sd} (T_F^s - T_F^d) = - \left(\frac{\partial \hat{h}_F^s}{\partial p_F^s} \right)_{T_F^s} \left[(A\rho)_F^s \frac{\partial p_F^s}{\partial t} + \dot{m}_F^s \frac{\partial p_F^s}{\partial x} \right], \quad 0 \leq x \leq H \quad (10)$$

For a 2-phase system (saturated water), temperature is considered as a function of pressure

$$T_F^s = T_F^s(p_F^s) \quad (11)$$

And the quality of the steam is used as an independent variable. The specific enthalpy of the water steam two-phase system can be expressed as a linear combination of specific enthalpy of water and specific enthalpy of steam. The weight function depends upon the quality of the steam. This relationship is given by

$$\hat{h}_F^s = \hat{h}_v^s \varepsilon_F^s + \hat{h}_l^s (1 - \varepsilon_F^s) \quad (12)$$

Moreover, the specific enthalpy of steam and water are functions of temperature themselves

$$\hat{h}_v^s = \hat{h}_v^s(T_F^s) \quad 13(a)$$

$$\hat{h}_l^s = \hat{h}_l^s(T_F^s) \quad 13(b)$$

So equation (12) gives the specific enthalpy of the steam at a given temperature. Similarly the density of the steam can be determined by following relationships for a given temperature of steam

$$\rho_F^s = \rho_v \varepsilon_F^s + \rho_l (1 - \varepsilon_F^s) \quad (14)$$

$$\rho_v = \rho_v(T_F^s) \quad (15(a))$$

$$\rho_l = \rho_l(T_F^s) \quad (15(b))$$

Since the enthalpy is a function of temperature and quality, the following relations hold good

$$\frac{\partial h_F^s}{\partial t} = \left(\frac{\partial h_F^s}{\partial T_F^s} \right)_{\varepsilon_F^s} \left(\frac{\partial T_F^s}{\partial t} \right) + \left(\frac{\partial h_F^s}{\partial \varepsilon_F^s} \right)_{T_F^s} \left(\frac{\partial \varepsilon_F^s}{\partial t} \right) \quad (16(a))$$

$$\frac{\partial h_F^s}{\partial x} = \left(\frac{\partial h_F^s}{\partial T_F^s} \right)_{\varepsilon_F^s} \left(\frac{\partial T_F^s}{\partial x} \right) + \left(\frac{\partial h_F^s}{\partial \varepsilon_F^s} \right)_{T_F^s} \left(\frac{\partial \varepsilon_F^s}{\partial x} \right) \quad (16(b))$$

Now by substituting Eq 12 in 2 and using 4, 16(a) & 16(b), the heat balance equation for a two phase system in the steam tube can be written as

$$\left[(A\rho C_p)_p^s + A_F^s \rho_F^s \left(\frac{\partial \hat{h}_F^s}{\partial T_F^s} \right)_{\varepsilon_F^s} \right] \frac{\partial T_F^s}{\partial t} + \dot{m}_F^s \left(\frac{\partial \hat{h}_F^s}{\partial T_F^s} \right)_{\varepsilon_F^s} \frac{\partial T_F^s}{\partial x} + (\sigma U)^{sd} (T_F^s - T_F^d) = - \left(\frac{\partial \hat{h}_F^s}{\partial \varepsilon_F^s} \right)_{T_F^s} \left[(A\rho)_F^s \frac{\partial \varepsilon_F^s}{\partial t} + \dot{m}_F^s \frac{\partial \varepsilon_F^s}{\partial x} \right], \quad 0 \leq x \leq H \quad (17)$$

where

$$\left(\frac{\partial \hat{h}_F^s}{\partial T_F^s} \right)_{\varepsilon_F^s} = \varepsilon_F^s \frac{d\hat{h}_v}{dT_F^s} + (1 - \varepsilon_F^s) \frac{d\hat{h}_l}{dT_F^s}, \quad 0 \leq x \leq H \quad (18)$$

$$\left(\frac{\partial \hat{h}_F^s}{\partial \varepsilon_F^s} \right)_{T_F^s} = (\hat{h}_v - \hat{h}_l) \quad (19)$$

3.3 Initial and Boundary Conditions

The partial differential equations are unsolvable without boundary conditions. The various initial and the boundary conditions used for the given model are described below

Initial Conditions

$$T_F^d(x,0) = T_E^0(x) \quad 0 \leq x \leq H \quad (20)$$

$$T_F^s(x,0) = T_E^0(x) \quad 0 \leq x \leq H \quad (21)$$

$$T_F^d(x,0) = T_E^0(x) \quad 0 \leq x \leq H \quad (22)$$

$$T_F^u(x,0) = T_E^0(2H-x) \quad H \leq x \leq 2H \quad (23)$$

Boundary Conditions

$$T_E(r_0, z, t) = T_F^u(2H-z, t) \quad 0 \leq z \leq H, t \geq 0 \quad (24)$$

$$T_E(r_0, z, t) = T_F^u(2H-z, t) \quad 0 \leq z \leq H+h, t \geq 0 \quad (25)$$

$$T_E(r, H+h, t) = T_E^0(H+h) \quad 0 \leq r \leq h, t \geq 0 \quad (26)$$

$$\frac{\partial T_E}{\partial r}(0, z, t) = 0 \quad H \leq z \leq H+h, t \geq 0 \quad (27)$$

$$\frac{\partial T_E}{\partial z}(r_0, 0, t) = 0 \quad r_0 \leq r \leq h, t \geq 0 \quad (28)$$

$$T_F^d(0, t) = T_E^0(0) \quad t \geq 0 \quad (29)$$

$$T_F^s(0, t) = T_0^s(0) \quad t \geq 0 \quad (30)$$

$$T_E(r, z, 0) = T_E^0(z) \quad 0 \leq z \leq H, r_0 \leq r \leq h \text{ and } H \leq z \leq H+h, 0 \leq r \leq h, t \geq 0 \quad (31)$$

$$\dot{m}_F^s(0, t) = \dot{m}_0^s(t) \quad t \geq 0 \quad (32)$$

$$\dot{m}_F^d(0, t) = \dot{m}_0^d(t) \quad t \geq 0 \quad (33)$$

$$T_F^u(H, t) = T_F^d(H, t) = T_F^s(H, t) \quad t \geq 0 \quad (34)$$

$$p_F^s(0, t) = p_0^s(t) \quad t \geq 0 \quad (35)$$

$$\varepsilon_F^s(0, t) = \varepsilon_0^s(t) \quad t \geq 0 \quad (36)$$

3.4 Non-Dimensionalization

For Non-Dimensionalization of the governing equations, following scales have been used

$$\theta = \frac{T - T_E^0(0)}{T_{max} - T_E^0(0)} = \frac{T - T_E^0(0)}{(\Delta T)_{max}}$$

$$r^* = \frac{r}{h}, \quad x^* = \frac{x}{H}$$

$$z^* = \begin{cases} \frac{z}{H} & 0 \leq z \leq H \\ 1 + \frac{z-H}{h} & H \leq z \leq H+h \end{cases}$$

$$t^* = \left(\frac{t}{h^2/\alpha} \right)$$

$$\alpha = \left(\frac{\kappa}{\rho C_P} \right)_E$$

The governing equations in their Non-Dimensional form are given by

$$\frac{\partial \theta}{\partial t^*} = \frac{1}{r^*} \frac{\partial}{\partial r^*} \left(r^* \frac{\partial \theta}{\partial r^*} \right) + \frac{1}{L^2} \frac{\partial^2 \theta_E}{\partial z^{*2}} \quad (37)$$

$$(f_p)^d \frac{\partial \theta_F^d}{\partial t^*} + \frac{(Pe)^d}{L} \frac{\partial \theta_F^d}{\partial x^*} + (\beta^*)^{ud} (\theta_F^d - \theta_F^u) + (\beta^*)^{sd} (\theta_F^d - \theta_F^s) = \Sigma^* \quad 0 \leq x^* \leq 1 \quad (38)$$

$$(f_p)^u \frac{\partial \theta_F^u}{\partial t^*} + \frac{(Pe)^u}{L} \frac{\partial \theta_F^u}{\partial x^*} + (\beta^*)^{ud} (\theta_F^u - \theta_F^d) = 2\pi r^* \left(r^* \frac{\partial \theta_E}{\partial r^*} \right) \Big|_{r^* = r_0^*} \quad 1 \leq x^* \leq 2 \quad (39)$$

$$(f_p)^s \frac{\partial \theta_F^s}{\partial t^*} + \frac{(Pe)^s}{L} \frac{\partial \theta_F^s}{\partial x^*} + (\beta^*)^{sd} (\theta_F^s - \theta_F^d) = (P^*)^s \quad 0 \leq x^* \leq 1 \quad (40)$$

where,

$$(f_p)^d = \frac{(A\rho C_P)_p^d}{(A\rho C_P)_F^d} + 1 \quad (41)$$

$$(f_p)^\mu = \frac{(A\rho C_P)_p^\mu + (A\rho C_P)_F^\mu}{(A\rho C_P)_F^d} \quad (42)$$

$$(f_p)^s = \frac{(A\rho C_P)_p^s + A_F^s p_F^s \left(\frac{\partial \hat{h}_F^s}{\partial T_F^s} \right)}{(A\rho C_P)_F^d} p_F^s \quad (43)$$

$$(f_p)^s = \frac{(A\rho C_P)_p^s + A_F^s \varepsilon_F^s \left(\frac{\partial \hat{h}_F^s}{\partial T_F^s} \right)}{(A\rho C_P)_F^d} \varepsilon_F^s \quad (44)$$

$$(Pe)^d = \frac{h \dot{m}_F^d}{\alpha (A\rho)_F^d} \quad (45)$$

$$(Pe)^u = \frac{h \left(\dot{m} C_P \right)_F^u}{\alpha (A\rho C_P)_F^d} \quad (46)$$

$$(Pe)^s = \frac{h \dot{m}_F^s \left(\frac{\partial \hat{h}_F^s}{\partial T_F^s} \right)}{\alpha (A\rho C_P)_F^d} p_F^s \quad \text{for single phase} \quad (47)$$

$$(Pe)^s = \frac{h \dot{m}_F^s \left(\frac{\partial \hat{h}_F^s}{\partial T_F^s} \right)}{\alpha (A\rho C_P)_F^d} \varepsilon_F^s \quad \text{for two phase} \quad (48)$$

$$(\beta^*)^{ud} = \frac{h^2 (\sigma U)^{ud}}{\alpha (A \rho C_P)_F^d} \quad (49)$$

$$(\beta^*)^{sd} = \frac{h^2 (\sigma U)^{sd}}{\alpha (A \rho C_P)_F^d} \quad (50)$$

$$\Sigma^* = \frac{h^2 S}{\alpha (\Delta T)_{max} (A \rho C_P)_F^d} \quad (51)$$

$$S = \left[\frac{\dot{m}_F^s \varepsilon_F^s (\hat{h}_v - \hat{h}_l)}{D} \right] (H - h, t) \quad (52)$$

$$\lambda = \frac{\kappa}{(A \rho C_P)_P^d} \quad (53)$$

$$\gamma^* = \frac{h^2 \kappa}{\alpha (A \rho C_P)_F^d} \quad (54)$$

$$(P^*)^s = -h^2 \left(\frac{\partial h_F^s}{\partial p_F^s} \right)_{T_F^*} \left[(A \rho)_F^s \frac{\partial p_F^s}{\partial t} + m_F^s \frac{\partial p_F^s}{\partial x} \right] \quad \text{for single phase} \quad (55)$$

$$(P^*)^s = -h^2 \left(\frac{\partial h_F^s}{\partial \varepsilon_F^s} \right)_{T_F^*} \left[(A \rho)_F^s \frac{\partial \varepsilon_F^s}{\partial t} + m_F^s \frac{\partial \varepsilon_F^s}{\partial x} \right] \quad \text{for two phase} \quad (56)$$

$$L = 1 \quad z^* \geq 1 \quad (57)$$

$$L = \frac{H}{h} \quad 0 \leq z^* \leq 1 \quad 0 \leq x^* \leq 2 \quad (58)$$

$$V^d = \frac{\dot{m}_F^d}{(A \rho)_F^d} \quad (59)$$

$$V^u = \frac{\left(\dot{m} C_P \right)_F^u}{(A \rho C_P)_F^d} \quad (60)$$

$$V^s = \frac{\dot{m}_F^s \left(\frac{\partial \hat{h}_F^s}{\partial T_F^s} \right)_{p_F^s}}{(A \rho C_P)_F^d} \quad \text{for single phase} \quad (61)$$

$$V^s = \frac{\dot{m}_F^s \left(\frac{\partial \hat{h}_F^s}{\partial T_F^s} \right)_{\varepsilon_F^s}}{(A \rho C_P)_F^d} \quad \text{for two phase} \quad (62)$$

Chapter 4

The Numerical Solution

The governing equations described in the previous chapter are non-linear partial differential equations. Generally, it is not possible to find a closed form solution for non-linear PDEs with given boundary conditions. So the governing equations are solved numerically with the boundary and initial conditions described in chapter 3.

Algebraic equations of the form $Ax=B$ are far easier to solve compared to PDEs. So the Numerical methods are used to reduce PDEs to algebraic equations. In this study we have used FEM for this purpose. The algebraic equations thus obtained are then solved to obtain the desired solution.

4.1 Spatial Descretization

The whole computational domain has been divided into four computational sub-domains; one for earth and rest for the reactor tubes. The computational domain for earth Ω_E can be descretized into sub-domains called elements given by Ω^e_E , $e = 1, 2, 3, \dots, nele_E$. The number of elements, $nele_E$ depends completely upon the physical set up of the problem and the desired accuracy of the solution. In the present study, the computational domain is rectangular in shape and the elements are also rectangular. The computational domains for the reactor tubes $\Omega_F^u, \Omega_F^s, \Omega_F^d$ are linear. So the elements of these domains are linear. Because of the difference in dimensions of the elements of earth computational domain and the reactor tubes computational domain, the implementation of various FEM techniques is very difficult. So for the reactor tubes computational domains, two-dimensional pseudo-elements have been used. Each pseudo-element consists of two one-dimensional elements facing each other. This has been depicted in figure 4.1

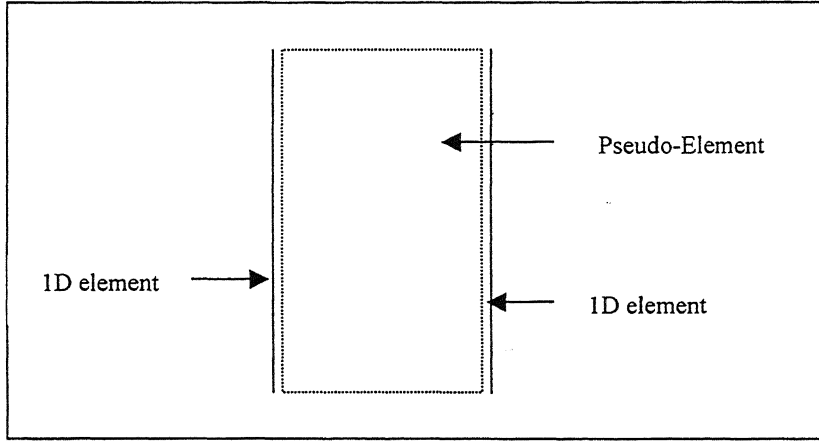


Figure 4.1 Two-dimensional Pseudo element

4.2 Variational Formulation

For setting up the variational formulation we need to define sets of weight functions and the solution functions. These finite dimensional spaces, can be defined as follows on the basis of the boundary conditions.

$$V^h(\Omega_E) = \left[w^h \mid w^h \in H^{1h}(\Omega_E), w^h = 0, \quad \text{on } \Gamma_g \right] \quad (63)$$

$$S^h(\Omega_E) = \left[\theta^h \mid \theta^h \in H^{1h}(\Omega_E), \theta_E^h = g, \quad \text{on } \Gamma_g \right] \quad (64)$$

The two spaces can be called as Variation Space and Solution space respectively.

The discrete variational formulation (Galerkin Formulation) associated with the heat conduction equation of earth can be given by the following equation

$$\int_{\Omega_E} w^h \frac{\partial \theta_E^h}{\partial t^*} r^* dr^* L dz^* + \int_{\Omega_E} \left(\frac{\partial w^h}{\partial r^*} \frac{\partial \theta_E^h}{\partial r^*} + \frac{1}{L^2} \frac{\partial w^h}{\partial z^*} \frac{\partial \theta_E^h}{\partial z^*} \right) r^* dr^* L dz^* = 0 \quad (65)$$

Here we wish to find all $\theta^h \in S^h$ by solving above equation such that $w^h \in V^h$

The heat flux at the up tube – Earth interface is approximated over a pseudo-element (shown in figure 4.2) as

$$2\pi\gamma^*\left(r^*\frac{\partial\theta_E}{\partial r^*}\right)\Big|_{r^*=r_0^*}=2\pi\gamma^*\left(r_0^*+\frac{\Delta r^*}{2}\right)\left(\frac{\theta^+-\theta}{\Delta r^*}\right) \quad (66)$$

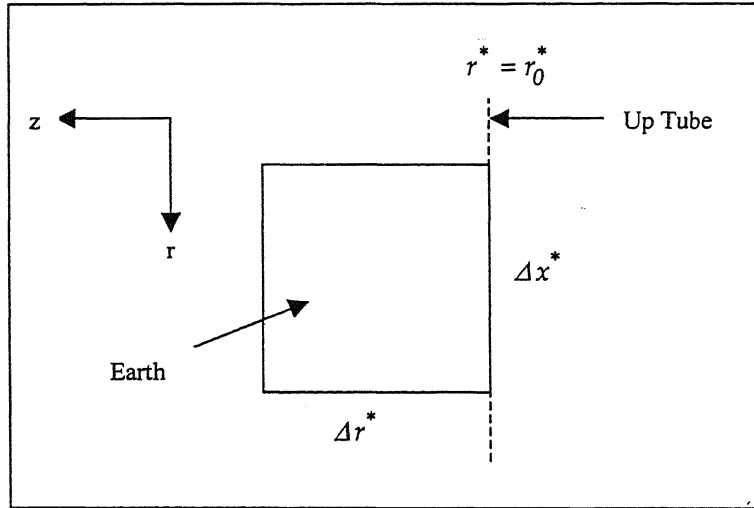


Figure 4.2 The Earth-Up tube interface

The computational domains for the reactor tubes or fluid can be defined as follows

$$\Omega_F^d = \left(x^* \mid 0 \leq x^* \leq 1\right) \quad 67(a)$$

$$\Omega_F^s = \left(x^* \mid 0 \leq x^* \leq 1\right) \quad 67(b)$$

$$\Omega_F^u = \left(x^* \mid 1 \leq x^* \leq 2\right) \quad 67(c)$$

The Variation and Solution spaces for these computational domains can be defined as follows

Down Tube

$$V^{dh}\left(\Omega_F^d\right)=\left[w^{dh} \mid w^{dh} \in H^{1h}\left(\Omega_F^d\right), w^{dh}=0 \text { at } x^*=0\right] \quad 68(a)$$

$$S^{dh}(\Omega_F^d) = \left[\theta_F^{dh} \mid \theta_F^{dh} \in H^{1h}(\Omega_F^d), \theta_F^{dh} = 0 \text{ at } x^* = 0 \right] \quad (68(b))$$

Steam Tube

$$V^{sh}(\Omega_F^s) = \left[w^{sh} \mid w^{sh} \in H^{1h}(\Omega_F^s), w^{sh} = 0 \text{ at } x^* = 0 \right] \quad (69(a))$$

$$S^{sh}(\Omega_F^s) = \left[\theta_F^{sh} \mid \theta_F^{sh} \in H^{1h}(\Omega_F^s), \theta_F^{sh} = \theta_o^s(t) \text{ at } x^* = 0 \right] \quad (69(b))$$

Up Tube

$$V^{uh}(\Omega_F^u) = \left[w^{uh} \mid w^{uh} \in H^{1h}(\Omega_F^u) \right] \quad (70(a))$$

$$S^{uh}(\Omega_F^u) = \left[\theta_F^{uh} \mid \theta_F^{uh} \in H^{1h}(\Omega_F^u) \right] \quad (70(b))$$

To ensure proper heat transfer at the bottom of the reactor, the Solution Space has to satisfy following constraint

$$\theta_F^{sh} = \theta_F^{dh} = \theta_F^{uh} \quad \text{at } x^* = 1, \forall t \geq 0 \quad (71)$$

The Galerkin discrete variational form is known to generate spurious node-to-node oscillations for convective equations. So for the convective heat balance equations for the reactor tubes Petrov-Galerkin method has been used. The variational forms associated with these equations (38, 39 and 40) are given by

Down Tube

$$\begin{aligned} \int_{\Omega_F^d} \left(w^{dh} + \delta^{dh} \right) \left[(f_p)^d \frac{\partial \theta_F^{dh}}{\partial t^*} + \frac{(Pe)^d}{L} \frac{\partial \theta_F^{dh}}{\partial x^*} + (\beta^*)^{ud} (\theta_F^{dh} - \theta_F^{uh}) \right. \\ \left. + (\beta^*)^{sd} (\theta_F^{dh} - \theta_F^{sh}) \right] d\Omega = \int_{\Omega_F^d} \left(w^{dh} + \delta^{dh} \right) \Sigma^* d\Omega, \quad \forall w^{th} \in V^{dh} \end{aligned} \quad (72)$$

Up Tube

$$\int_{\Omega_F^u} \left(w^{uh} + \delta^{uh} \right) \left[\left(f_p \right)^u \frac{\partial \theta_F^{uh}}{\partial t^*} + \frac{(Pe)^u}{L} \frac{\partial \theta_F^{uh}}{\partial x^*} + \left(\beta^* \right)^{ud} \left(\theta_F^{uh} - \theta_F^{dh} \right) \right. \\ \left. + 2\pi\gamma^* \left(r_0^* - \frac{\Delta r^*}{2} \right) \left(\frac{\theta_F^{uh} - \left(\theta^* \right)^h}{2} \right) \right] d\Omega = 0 \quad (73)$$

Steam Tube

$$\int_{\Omega_F^s} \left(w^{sh} + \delta^{sh} \right) \left[\left(f_p \right)^s \frac{\partial \theta_F^{sh}}{\partial t^*} + \frac{(Pe)^s}{L} \frac{\partial \theta_F^{sh}}{\partial x^*} + \left(\beta^* \right)^{sd} \left(\theta_F^{sh} - \theta_F^{dh} \right) \right] d\Omega \\ = \int_{\Omega_F^s} \left(w^{sh} + \delta^{sh} \right) \left(P^* \right)^s d\Omega \quad (74)$$

Where δ^h is the Petrov-Galerkin supplement function and it is defined as

$$\delta^h = C_{2r} \frac{\Delta x^*}{2} \text{sign} \left(\frac{Pe}{f_p} \right) \frac{\partial w^h}{\partial x^*} \quad (75)$$

Where C_{2r} is the Courant number. For this study, Courant number is unity

$$C_{2r} = 1 \quad (76)$$

Using the value of Courant number and writing the differential in the local coordinate reduces the supplement function to

$$\delta^h = \text{sign} \left(\frac{Pe}{f_p} \right) \frac{\partial w^h}{\partial \xi} \quad (77)$$

$$\text{Let } c = \text{sign} \left(\frac{Pe}{f_p} \right)$$

So, finally,

$$\delta^h = c \frac{\partial w^h}{\partial \xi} \quad (78)$$

4.3 Elemental Matrices

The variational formulation of the governing equations of the reactor tubes gives rise to the elemental matrices. The elemental heat capacity matrices, convection matrices and matrices corresponding to the heat exchange terms are given by

$$(C_F^e)^{sd} = \frac{\Delta x^*}{2} \begin{vmatrix} (f_p)_1 \left(\frac{1-c}{2} - \frac{c}{3} \right) + (f_p)_4 \left(\frac{1-c}{6} - \frac{c}{6} \right) & 0 & 0 & (f_p)_1 \left(\frac{1-c}{6} - \frac{c}{6} \right) + (f_p)_4 \left(\frac{1-c}{2} - \frac{c}{3} \right) \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ (f_p)_1 \left(\frac{1+c}{6} + \frac{c}{3} \right) + (f_p)_4 \left(\frac{1+c}{6} + \frac{c}{6} \right) & 0 & 0 & (f_p)_1 \left(\frac{1+c}{2} + \frac{c}{3} \right) + (f_p)_4 \left(\frac{1+c}{6} + \frac{c}{6} \right) \end{vmatrix} \quad (79)$$

$$(K_F^e)^{sd} = \begin{vmatrix} (Pe)_1^s \left(-\frac{1}{3} - \frac{c}{4} \right) + (Pe)_4^s \left(-\frac{1}{6} + \frac{c}{4} \right) & 0 & 0 & (Pe)_1^s \left(\frac{1}{3} - \frac{c}{4} \right) + (Pe)_4^s \left(\frac{1}{6} - \frac{c}{4} \right) \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ (Pe)_1^s \left(-\frac{1}{6} - \frac{c}{4} \right) + (Pe)_4^s \left(-\frac{1}{3} - \frac{c}{4} \right) & 0 & 0 & (Pe)_1^s \left(\frac{1}{6} + \frac{c}{4} \right) + (Pe)_4^s \left(\frac{1}{3} + \frac{c}{4} \right) \end{vmatrix} \quad (80)$$

$$(K_F^e)^{sd} = \frac{\Delta x^*}{2} (\beta^*) \begin{vmatrix} \left(\frac{2-c}{3} - \frac{c}{2} \right) & -\left(\frac{2-c}{3} - \frac{c}{2} \right) & -\left(\frac{1-c}{3} - \frac{c}{2} \right) & \left(\frac{1-c}{3} - \frac{c}{2} \right) \\ -\left(\frac{2+c}{3} + \frac{c}{2} \right) & \left(\frac{2+c}{3} + \frac{c}{2} \right) & \left(\frac{1+c}{3} + \frac{c}{2} \right) & -\left(\frac{1+c}{3} + \frac{c}{2} \right) \\ -\left(\frac{1-c}{3} - \frac{c}{2} \right) & \left(\frac{1-c}{3} - \frac{c}{2} \right) & \left(\frac{2-c}{3} - \frac{c}{2} \right) & -\left(\frac{2-c}{3} - \frac{c}{2} \right) \\ \left(\frac{1+c}{3} + \frac{c}{2} \right) & -\left(\frac{1+c}{3} + \frac{c}{2} \right) & -\left(\frac{2+c}{3} + \frac{c}{2} \right) & \left(\frac{2+c}{3} + \frac{c}{2} \right) \end{vmatrix} \quad (81)$$

The elemental force vector due to heat source in up and down tubes are given by

$$(f_F^e)^{ud} = \frac{\Delta x^*}{2} \begin{vmatrix} \left(\frac{2-c}{3} - \frac{c}{2} \right) \Sigma_1^* + \left(\frac{1-c}{3} - \frac{c}{2} \right) \Sigma_4^* \\ \left(\frac{2+c}{3} + \frac{c}{2} \right) \Sigma_2^* + \left(\frac{1+c}{3} + \frac{c}{2} \right) \Sigma_3^* \\ \left(\frac{1-c}{3} - \frac{c}{2} \right) \Sigma_2^* + \left(\frac{2-c}{3} - \frac{c}{2} \right) \Sigma_3^* \\ \left(\frac{1+c}{3} + \frac{c}{2} \right) \Sigma_1^* + \left(\frac{2+c}{3} + \frac{c}{2} \right) \Sigma_4^* \end{vmatrix} \quad (82)$$

The elemental force vector for the steam tube is given by

$$\begin{pmatrix} f_F^e \end{pmatrix}^{sd} = \frac{\Delta x^*}{2} \begin{bmatrix} \left(\frac{2}{3} - \frac{c}{2} \right) (P^*)_1^s + \left(\frac{1}{3} - \frac{c}{2} \right) (P^*)_4^s \\ 0 \\ 0 \\ \left(\frac{1}{3} + \frac{c}{2} \right) (P^*)_1^s + \left(\frac{2}{3} + \frac{c}{2} \right) (P^*)_4^s \end{bmatrix} \quad (83)$$

4.4 Assembly

The assembly procedure is described by the following equations

$$C = {}_e \in E_E^A C_E^e + {}_e \in E_F^A \left[(C_F^e)^{ud} + (C_F^e)^{sd} \right] \quad (84)$$

$$K = {}_e \in E_E^A K_E^e + {}_e \in E_F^A \left[(K_F^e)^{ud} + (K_F^e)^{ud} + (K_F^e)^{sd} + (K_F^e)^{sd} \right] + {}_e \in E_A^A K_F^{e''} \quad (85)$$

$$F = {}_e \in E_E^A f_E^e + {}_e \in E_F^A \left[(f_F^e)^{ud} + (f_F^e)^{sd} \right] \quad (86)$$

4.5 Solution of the simplified equations

The assembly of the elemental matrices leads to a set of time-dependent ordinary differential equations.

$$\begin{aligned} C \frac{\partial d}{\partial t} + Kd &= F \\ d(0) &= 0 \end{aligned} \quad (87)$$

Or,

$$Cv + Kd = F \quad 88(a)$$

$$d(0) = 0 \quad 88(b)$$

This system of equations has been solved using Predictor–Multicorrector method. The solution procedure has been described below

The solution for $n+1$ th step is predicted by

$$p_{n+1} = d_n + (1-\lambda) t v_n \quad (89)$$

And corrected by

$$d_{n+1} = p_{n+1} + \lambda t v_{n+1} \quad (90)$$

Where

$$v_{n+1} = (C_{n+1} + \lambda t K_{n+1})^{-1} (F_{n+1} - K_{n+1} p_{n+1}) \quad (91)$$

Chapter 5

Results and Discussion

The start-up of the reactor is studied for the case when hot water is introduced in the steam tube. The following numerical quantities were used to set up the physical problem

$$r_0 = 0.52 \text{ ft}$$

$$H = 5000 \text{ ft}$$

$$h = 10 \text{ ft}$$

$$T_E^0(z) = 80 + 0.628z \text{ } ^\circ\text{F}$$

$$(\rho C_P)_E = 40 \text{ BTU/ft}^3$$

$$(A)_P^d = 0.037601277 \text{ ft}^2$$

$$(A)_P^u = 0.097555518 \text{ ft}^2$$

$$(A)_P^s = 0.012271846 \text{ ft}^2$$

$$(A)_F^d = 0.132822283 \text{ ft}^2$$

$$(A)_F^u = 0.20141904 \text{ ft}^2$$

$$(A)_F^s = 0.021816615 \text{ ft}^2$$

$$(A\rho C_P)_F^d = 8.234981546 \text{ BTU/ft } ^\circ\text{F}$$

$$\sigma^{ud} = 1.65915362 \text{ ft}^2/\text{ft}$$

$$\sigma^{sd} = 0.916297857 \text{ ft}^2/\text{ft}$$

$$\beta_{sd}^d = 1201.5341$$

$$\beta_{sd}^s = 2.748893571$$

$$\gamma^* = 71.8614893$$

$$f_P^d = 0.160667625$$

$$f_p^u = 0.416847903$$

$$f_p^s = 0.052436739$$

A mesh of 2813 nodes, 2536 two-dimensional elements and 228 one dimensional elements (152 pseudo-elements) has been used to discretize the computational domain which is a rectangle. The total number of 2688 two-dimensional elements has been used.

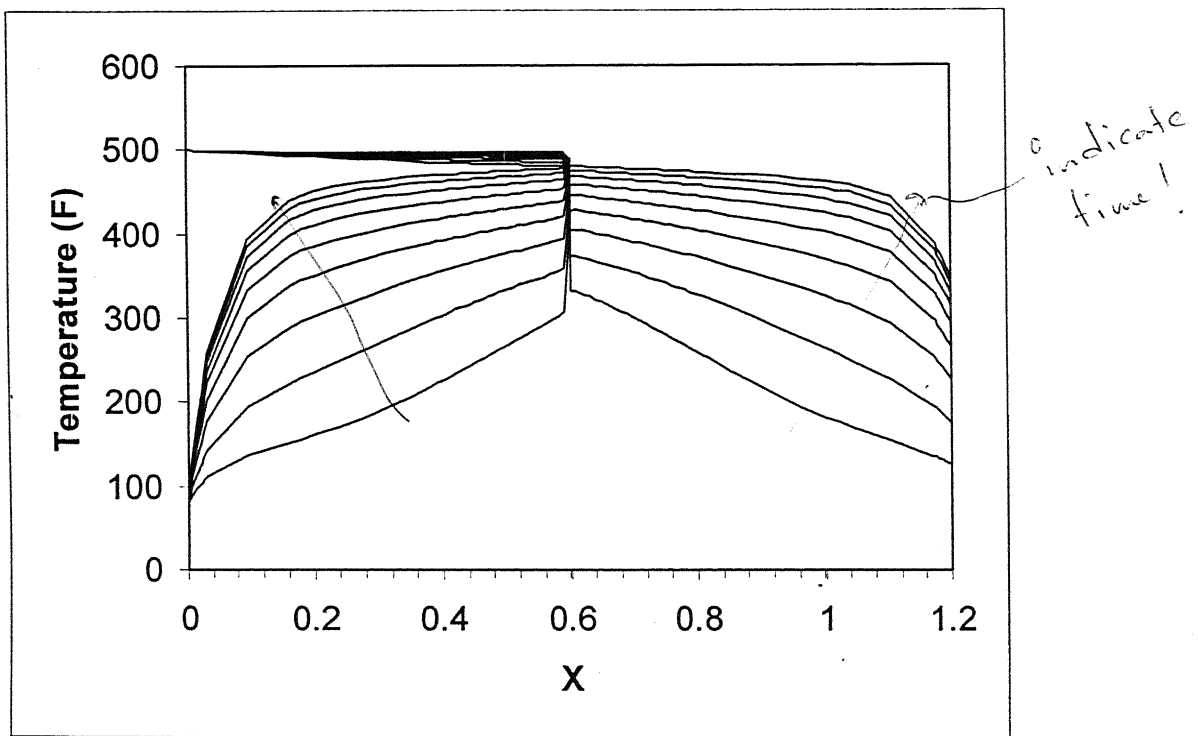


Figure 5.1 Temperature Profile of the tubes after 12 hours

The reactor was started up by introducing hot water at 500 °F and 700 bars through the steam tube. Actually the temperature at the inlet of the steam tube has been ramped up from 50 °F to 500 °F in 1.2 hours. The mass flow rate at the inlet of steam tube is assumed to be 100,000 Kg/s and inlet of down tube as 50,000 Kg/s. Figure 5.1 shows the temperature profile of the tubes after 12 hours of introduction of water. This temperature profile is in agreement with the previous work [1].

The bottom temperature (bottom of the reactor tubes) is a parameter to determine the time to start up the reaction. Hot water continues through steam tube for that time only for which the bottom temperature has not reached the desired initiation temperature of the reaction. Once the initiation temperature is reached, hot water supply is shut off and oxygen supply is started. The bottom temperature variation for 12 hours is shown in figure 5.2. The bottom temperature first decreases rapidly, then increases sharply and finally becomes almost constant. The final bottom temperature is very close to the inlet temperature of the steam tube.

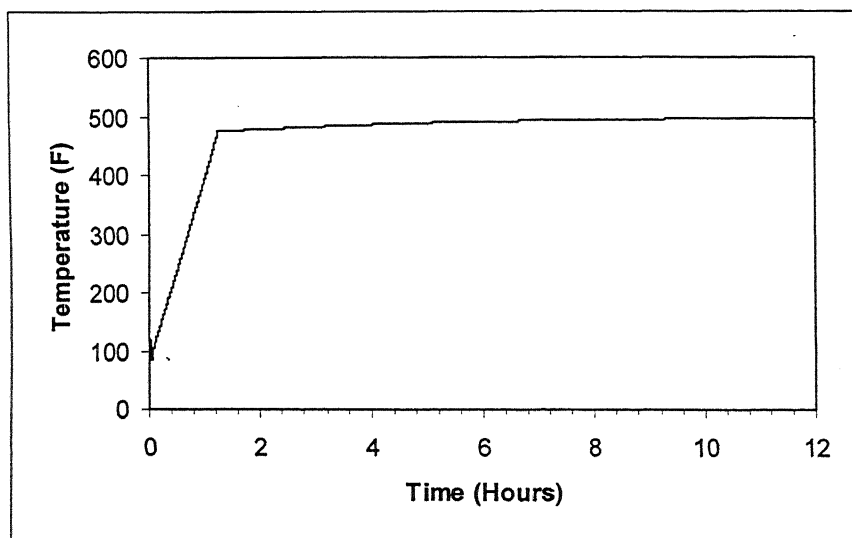


Figure 5.2
Bottom Temperature Vs Time

The fall and rise of the bottom temperature has been captured in figure 5.3

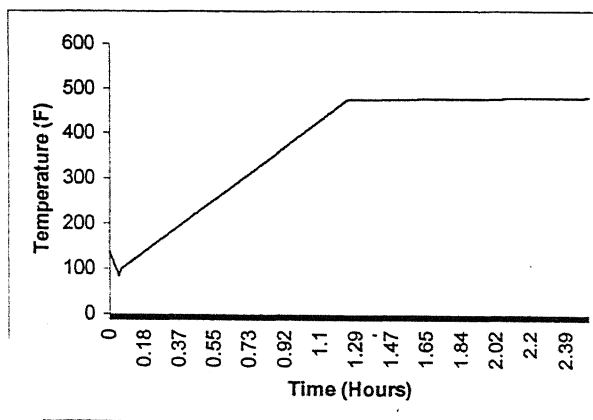


Figure 5.3 Bottom Temperature Vs Time:
Initial part of the curve

Again the variation of the temperature is same as found by Mittal S. (1990). Another important parameter to study is the temperature of the fluid at the exit of up tube. It is a measure of actual heat transfer from fluid to earth. The exit temperature increases constantly with the time as heat is being added to the system through the inlet of the steam tube constantly. After a long time, at steady state, it becomes flat. Figure 5.4 shows how the exit temperature varies with time.

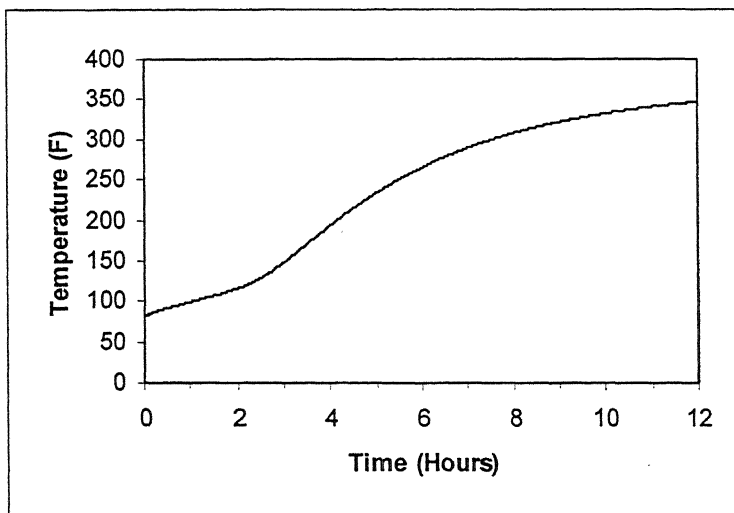


Figure 5.4 Exit Temperature Vs Time

The exit temperature variation is also found to be the same as the previous study [1].

Chapter 6

Numerical aspects of the Wet-Oxidation Reaction

Once the reactor is heated to the desired value of bottom temperature, the hot water/steam supply is stopped and the oxygen supply is opened. The oxidation reaction of the sludge is exothermic in nature; the heat produced by the reaction carries on the process further. In this chapter, a possible method for the numerical study of the reaction has been suggested.

6.1 Governing Equations

The governing equations of the fluid described in chapter 3 still apply but now we will have conservation of species law in addition to the conservation of mass, momentum and energy.

Let \dot{m}_d be the total mass flow rate in the down tube. The mass flow rate \dot{m}_i and mass fraction ω_i of the i^{th} species are related as

$$\dot{m}_i = \dot{m}_d \omega_i$$

Let ρ be the local fluid density, ρ_i and r_i be the density and rate of production of i^{th} species. So,

$$\rho_i = \rho \omega_i$$

If A_d is the area of cross section of the down tube then the continuity equation for the i^{th} species is given by

$$A_d \frac{\partial}{\partial t} (\rho \omega_i) + \frac{\partial}{\partial z} (\dot{m}_d \omega_i) = A_d r_i$$

The Total Continuity equation will be the sum of the continuity equations of all the species. Since $\sum_i \omega_i = 1$, the Total Continuity Equation then becomes

$$A_d \frac{\partial \rho}{\partial t} + \frac{\partial \dot{m}_o}{\partial z} = 0$$

Since very dilute sludge is used in Deep Well Wet Oxidation Process, it is reasonable to assume that the local density of the fluid does not vary much with respect to time i.e. $\frac{\partial \rho}{\partial t} \approx 0$. The Total Continuity Equation then becomes

$$\frac{\partial \dot{m}_i}{\partial z} \approx 0$$

i.e. the axial variation of the mass flow rate of the i^{th} species is negligible. In fact the axial variation of mass flow rates of all the species would be negligible. If there are $N-1$ species then for the i^{th} species the continuity equation becomes

$$\rho \frac{\partial \omega_i}{\partial t} + \frac{\dot{m}_o}{A_d} \frac{\partial \omega_i}{\partial z} = r_i, i=1,2,\dots,N-1$$

At the bottom of the reactor continuity is assured by

$$\dot{m}_u = \dot{m}_d + \dot{m}_{o_2}$$

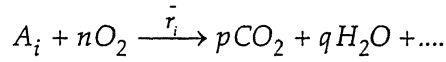
The continuity equation in the up tube is given by

$$\rho \frac{\partial \omega_i}{\partial t} + \frac{\dot{m}_u}{A_u} \frac{\partial \omega_i}{\partial z} = r_i, i=1,2,\dots,N-1$$

Where, A_u is the area of the up tube.

6.2 The Reaction Kinetics

The rate of reaction for the i^{th} species depends upon the mass fraction of that species, mass fraction of oxygen and the Temperature field. The oxidation reaction of the i^{th} species can be given as



Since this is an exothermic reaction, the heat of reaction would be negative. The continuity equation of the i^{th} species is given by

$$\rho \frac{\partial \omega_i}{\partial t} + \frac{\dot{m}_T}{A} \frac{\partial \omega_i}{\partial z} = r_i$$

Where, A is area of up or down tube and \dot{m}_T is the local mass flow rate. The rate of reaction is given by

$$r_i = -n_i k_0 e^{-\frac{E}{RT}} \prod_{i=1}^N \omega_i^{p_i}$$

Therefore, the continuity equation becomes

$$\rho \frac{\partial \omega_i}{\partial t} + \frac{\dot{m}_T}{A} \frac{\partial \omega_i}{\partial z} = -n_i k_0 e^{-\frac{E}{RT}} \prod_{j=1}^N w_j^{p_j}$$

or,

$$\rho \frac{\partial \omega_i}{\partial t} + \frac{\dot{m}_T}{A} \frac{\partial \omega_i}{\partial z} + \left(n_i k_0 e^{-\frac{E}{RT}} \prod_{j=1}^N w_j^{p_j} \omega_i^{p_i-1} \right) \omega_i = 0$$

or,

$$\rho \frac{\partial \omega_i}{\partial t} + \frac{\dot{m}_T}{A} \frac{\partial \omega_i}{\partial z} + Q_i \omega_i = 0$$

where,

$$Q_i = n_i k_0 e^{-\frac{E}{RT}} \prod_{j=1}^N w_j^{p_j} \omega_i^{p_i-1}$$

6.3 Variational Formulation

The spatial discretization remains same as described in chapter 4. The Galerkin variational form can be used for the additional governing equations. The various

elemental matrices for a pseudo-element formed by one-dimensional real elements of up and down tube can be thus obtained as

$$= \begin{vmatrix} \frac{\Delta s}{2} \left[\rho_1 \left(\frac{1}{2} - \frac{c}{3} \right) + \rho_4 \left(\frac{1}{6} - \frac{c}{6} \right) \right] & 0 & 0 & \frac{\Delta s}{2} \left[\rho_1 \left(\frac{1}{6} - \frac{c}{6} \right) + \rho_4 \left(\frac{1}{6} - \frac{c}{3} \right) \right] \\ 0 & \frac{\Delta s}{2} \left[\rho_3 \left(\frac{1}{6} + \frac{c}{6} \right) + \rho_2 \left(\frac{1}{2} + \frac{c}{3} \right) \right] & \frac{\Delta s}{2} \left[\rho_3 \left(\frac{1}{6} + \frac{c}{3} \right) + \rho_2 \left(\frac{1}{6} + \frac{c}{6} \right) \right] & 0 \\ 0 & \frac{\Delta s}{2} \left[\rho_3 \left(\frac{1}{6} - \frac{c}{6} \right) + \rho_2 \left(\frac{1}{6} - \frac{c}{3} \right) \right] & \frac{\Delta s}{2} \left[\rho_3 \left(\frac{1}{2} - \frac{c}{3} \right) + \rho_2 \left(\frac{1}{6} - \frac{c}{6} \right) \right] & 0 \\ \frac{\Delta s}{2} \left[\rho_1 \left(\frac{1}{6} + \frac{c}{3} \right) + \rho_4 \left(\frac{1}{6} + \frac{c}{6} \right) \right] & 0 & 0 & \frac{\Delta s}{2} \left[\rho_1 \left(\frac{1}{6} + \frac{c}{6} \right) + \rho_4 \left(\frac{1}{6} + \frac{c}{3} \right) \right] \end{vmatrix}$$

$$k = \begin{vmatrix} k_{11} & 0 & 0 & k_{14} \\ 0 & k_{22} & k_{23} & 0 \\ 0 & k_{32} & k_{33} & 0 \\ k_{41} & 0 & 0 & k_{44} \end{vmatrix}$$

Where,

$$k_{11} = \frac{\Delta s}{2} \left[Q_1^i \left(\frac{1}{2} - \frac{c}{3} \right) + Q_4^i \left(\frac{1}{6} - \frac{c}{6} \right) \right] + \frac{1}{A} \left[\left(-\frac{1}{3} + \frac{c}{4} \right) \dot{m}_1 + \left(-\frac{1}{6} + \frac{c}{4} \right) \dot{m}_4 \right]$$

$$k_{14} = \frac{\Delta s}{2} \left[Q_1^i \left(\frac{1}{6} - \frac{c}{6} \right) + Q_4^i \left(\frac{1}{6} - \frac{c}{3} \right) \right] + \frac{1}{A} \left[\left(\frac{1}{3} - \frac{c}{4} \right) \dot{m}_1 + \left(\frac{1}{6} - \frac{c}{4} \right) \dot{m}_4 \right]$$

$$k_{14} = \frac{\Delta s}{2} \left[Q_1^i \left(\frac{1}{6} + \frac{c}{6} \right) + Q_4^i \left(\frac{1}{6} + \frac{c}{3} \right) \right] + \frac{1}{A} \left[\left(-\frac{1}{6} - \frac{c}{4} \right) \dot{m}_1 + \left(-\frac{1}{3} - \frac{c}{4} \right) \dot{m}_4 \right]$$

$$k_{44} = \frac{\Delta s}{2} \left[Q_1^i \left(\frac{1}{6} + \frac{c}{3} \right) + Q_4^i \left(\frac{1}{2} + \frac{c}{3} \right) \right] + \frac{1}{A} \left[\left(\frac{1}{6} + \frac{c}{4} \right) \dot{m}_1 + \left(\frac{1}{3} + \frac{c}{4} \right) \dot{m}_4 \right]$$

$$k_{22} = \frac{\Delta s}{2} \left[Q_3^i \left(\frac{1}{6} + \frac{c}{6} \right) + Q_2^i \left(\frac{1}{2} + \frac{c}{3} \right) \right] + \frac{1}{A} \left[\left(\frac{1}{6} + \frac{c}{4} \right) \dot{m}_3 + \left(\frac{1}{3} + \frac{c}{4} \right) \dot{m}_2 \right]$$

$$k_{23} = \frac{\Delta s}{2} \left[Q_3^i \left(\frac{1}{6} + \frac{c}{3} \right) + Q_2^i \left(\frac{1}{6} + \frac{c}{6} \right) \right] + \frac{1}{A} \left[\left(-\frac{1}{6} - \frac{c}{4} \right) \dot{m}_3 + \left(-\frac{1}{3} - \frac{c}{4} \right) \dot{m}_2 \right]$$

$$k_{32} = \frac{\Delta s}{2} \left[Q_3^i \left(\frac{1}{6} - \frac{c}{6} \right) + Q_2^i \left(\frac{1}{6} - \frac{c}{3} \right) \right] + \frac{1}{A} \left[\left(\frac{1}{3} - \frac{c}{4} \right) \dot{m}_3 + \left(\frac{1}{6} - \frac{c}{4} \right) \dot{m}_2 \right]$$

$$k_{33} = \frac{\Delta s}{2} \left[Q_3^i \left(\frac{1}{2} - \frac{c}{3} \right) + Q_2^i \left(\frac{1}{6} - \frac{c}{6} \right) \right] + \frac{1}{A} \left[\left(-\frac{1}{3} + \frac{c}{4} \right) \dot{m}_3 + \left(-\frac{1}{6} + \frac{c}{4} \right) \dot{m}_2 \right]$$

The elemental force vector becomes,

$$f = \begin{bmatrix} \left(\frac{2}{3} - \frac{c}{2} \right) f_1 + \left(\frac{1}{3} - \frac{c}{2} \right) f_4 \\ \left(\frac{1}{3} + \frac{c}{2} \right) f_3 + \left(\frac{2}{3} + \frac{c}{2} \right) f_2 \\ \left(\frac{2}{3} - \frac{c}{2} \right) f_3 + \left(\frac{1}{3} - \frac{c}{2} \right) f_2 \\ \left(\frac{1}{3} + \frac{c}{2} \right) f_1 + \left(\frac{2}{3} + \frac{c}{2} \right) f_4 \end{bmatrix}$$

The assembly procedure described in chapter 4 applies here too.

Chapter 7

Conclusion and Further Scope

7.1 Conclusion

The Finite model uses Galerkin formulation for the heat conduction equation for earth and Petrov-Galerkin formulation for the convection equations of the reactor tubes. It uses the Predictor-Multicorrector algorithm for solving the time dependent ordinary differential equations for a more accurate solution.

The model can be used to depict the time required for start up of the reactor and mass flow rate of the water required for a desired starting temperature. This model can also be used for comparing different geometries of reactors and efficiency of the reactor for different fluids.

The results obtained here are in agreement with the results of the previous study made by Mittal S (1990), within the machine generated computational error, as different machines were used for simulation.

7.2 Further Scope

This study can be carried forward with making some generalization. The friction in the pipe has been neglected here. The friction can be included, and then the pressure no longer is hydrostatic. Also, the properties of fluid in the down and up tubes can be assumed to be varying with temperature and pressure.

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